“Synthesis and Characterization of Fe and Mg doped Zinc Oxide nanostructured Thin Films”

A Synopsis of Ph.D. in Physics Subject

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➢ Introduction:-

Thin film is a layer of material ranging from fraction of a nanometer to few micrometers in thickness. Thin films have very interesting properties that are quite different from bulk materials. ZnO alloy is one of the most attractive metal oxides for photonic and electronic applications due to its unique properties such as wide band gap, large exciton binding energy, large saturation velocity and a high breakdown voltage. It is relatively cheap and non-toxic. At room temperature, it may be a new potential candidate for optoelectronic devices such as UV laser, blue light emitting diodes etc.

In this work, ZnO nano-petals on microscope glass substrates have been synthesized by using a modified aqueous chemical growth method and characterization like morphological, structural, optical and electrical can be studied.

Zinc oxide (ZnO) thin film is the II-IV thin film semiconductor which is widely used in many important applications such as sensors, photodetectors, LEDs, transistors and also as a conductive layer in the solar cells. As a conductive layer, ZnO thin film has band gap and resistivity of 3.35 eV and 4.4×10^{-3} Ω-cm respectively. ZnO can be fabricated by vacuum and non-vacuum processes and both methods have their own advantages.

In the current investigation, chemical spray pyrolysis technique will be used to create Fe and Mg-doped zinc oxide nanostructured thin films. This approach is cost-effective and time-saving.

Iron doped zinc oxide (ZnO:Fe) thin films were synthesized by changing the doping concentration between 0 and 6 at.% at a constant substrate temperature of 400°C. Analysis and discussion were conducted on the impact of Fe-doping concentration on the physical behavior of ZnO thin films. X-ray diffraction (XRD) patterns revealed the hexagonal wurtzite crystal structure.

Mg-doped zinc oxide thin films (MZO) have been researched and produced utilizing a straightforward spray pyrolysis process. X-ray diffraction (XRD) analysis supported the hexagonal Wurtzite structure of the ZnO thin films. Atomic force microscopy (AFM) was used to analyze the thin film's morphology. Utilizing ultraviolet-visible (UV-Vis) spectrophotometry and Hall Effect measurements for electrical characteristics, the optical qualities were carefully examined. AFM data show qualitatively and quantitatively how the

surface characteristics (topography, roughness) change with Mg content. According to the optical characterization, the optical band gap energy of MZO thin films increased from 3.20 to 3.43 (eV), and the transmittance rose from 75 to almost 90%.

➢ Literature Survey:-

T. Srinivasulu et al. [1] investigated Fe-doped ZnO thin films which have been synthesized by using spray pyrolysis technique. The as-grown Fe-doped ZnO films found to have a hexagonal wurtzite crystal structure. The evaluated band gap of the Fe-doped ZnO films decreased from 3.24 eV to 3.01 eV. The films with lower Fe-doping concentration less than 2 at. % showed higher transmittance and wider band gap compared to pure and highly Fe-doped ZnO films. Prepared films exhibited ferromagnetic behavior at room temperature.

Rujuta Lehru et al. [2] studied the electrical characteristics of Fe-doped ZnO nanostructured thin films produced by sol-gel Method. The role of grain boundaries to the conduction mechanism is shown by impedance spectroscopy studies. Based on correlations between structural features and electrical properties, it is possible to understand how temperature and magnetic field affect the samples' electrical properties. The secondary phase that results from Fe doping in ZnO impacts the sample's crystallinity and dielectric behavior. Fe-O bonds in the structure improve the structure's dielectric properties. With respect to Fe concentration and frequency, the maximum barrier height and dielectric constant values change.

D. Selloum et al. [3] synthesized the Fe-doped zinc oxide nanorods on ITO substrates take on several structural shapes. Variations in the optical band gap and carrier density of the ZnO films were caused by the addition of Fe dopant up to 4 at.%. For photoelectric applications, the physicochemical properties of semiconductors have been altered using a variety of dopants, including Cu, Sn, In, Cd, and Al. This study looked into the usage of hydrogen peroxide (H_2O_2) as a precursor for electrodeposition of doped ZnO. Although the crystalline clarity of the ZnO films diminished with increasing Fe content. To calculate carrier density, the space charge capacitance and photocurrent were measured.

Md Rahat Al Hassan et al. [4] expressed the synthesis of compositionally complex ZnO thin films doped with transition metals (Cr, Mn, Fe, Ni, and Cu). Compositionally complex ceramics (CCCs), a relatively novel idea in materials science, are ceramics that include several

dopants within the ZnO lattice. Due to the effects of particle agglomeration, adding dopants to ZnO films tends to increase the grain size. With increasing dopant concentration, the optical transmittance of the doped ZnO films changes, with some films exhibiting enhanced transmittance in the visible wavelength range.

P.L. Hadimani et al. [5] created Fe-doped ZnO thin films using the sol-gel spin coating technique. ZnO's crystallite size shrank with increasing Fe level, according to XRD measurements, and cubic spinel $ZnFe_2O_4$ was found in the sample with the highest Fe content. While SPM pictures demonstrated a decrease in surface roughness, FE-SEM micrographs showed a reduction in average particle size with increasing Fe content. The phase identification and particle size analysis were supported by TEM analysis. The samples were magnetized, as determined by VSM analysis, and the creation of ferromagnetic material at room temperature was confirmed by SQUID analysis. Measuring the electrical conductivity of the coatings revealed their semiconducting nature.

Hongtao Xu et al. [6] researched zinc oxide semiconductor for its resistance switching (RS) characteristics. With regard to programming speed, ON/OFF ratio, retention time, and reliability at high temperatures, ZnO-based RRAM devices have excelled. A difficulty in developing useful device applications is the dispersion of memory switching parameters, such as resistance values and switching voltages. To manage the positioning of conducting filaments (CFs) and stabilize the switching parameters, a variety of techniques, such as doping impurity elements and interfacial engineering, have been published.

Heri Sutanto et al. [7] deposited the Fe-doped ZnO (ZnO:Fe) thin films by sol-gel process and a spray-coating technique. The 20% Fe-doped ZnO thin film had the best performance for rhodamine b, methylene blue, and E. coli bacterium degradation, as well as the maximum transmittance and lowest energy band gap. The average particle size of the Fe-doped ZnO thin film was 333.75 nm, and it showed a root-like morphology with agglomeration and aggregation.

M. Rouchdi et al. [8] investigated the Mg-doped ZnO thin films produced using spray pyrolysis. Atomic force microscopy (AFM), which offered qualitative and quantitative data about the surface attributes, such as topography and roughness, was used to characterize the morphology of the thin films. Using UV-Vis spectrophotometry, the optical characteristics of the Mg-doped ZnO thin films were investigated, with results demonstrating a rise in

transmittance and optical band gap energy with increasing Mg content. Through Hall Effect measurements, the electrical characteristics of the thin films were examined.

Fayyaz Hussain et al. [9] expressed the structural, electronic, and optical properties of Mg-doped ZnO thin films. X-ray diffraction (XRD) measurements indicated that Mg doping increases the grain size of ZnO thin films. This increase in bandgap can be attributed to the introduction of new defects in the structure due to Mg doping. The increase in bandgap may result in a decrease in the carrier concentration of Mg-doped ZnO thin films.

P. Fermi Hilbert Inbaraj et al. [10] studied the deposition of pure and Mg-doped ZnO thin films using the CBD method. The Mg-doping results in an increase in the optical band gap. The transmittance of the films was over 90% in the visible region. The addition of Mg dopant ions in ZnO thin films increased the unit cell volume and caused a strained stress in the films. The Mg doped ZnO thin films exhibited a uniform and dense rod-like morphology. The optical energy gap of the films increased with an improvement in Mg doping concentrations.

➢ Motivation:-

1) Zinc oxide (ZnO) is one of the transparent conducting oxide (TCO) materials that have drawn a lot of interest due to its physical, chemical, optical and electrical characteristics.
2) ZnO is regarded as a strong choice for transparent electronic and optoelectronic applications in the near UV area including light-emitting diodes, laser diodes, gas sensors, and solar cells.
3) Thin films based on semiconductor metal oxides (SMOs) have been extensively used due to their distinct optical and electrical properties. Among all the SMOs, zinc oxide (ZnO) is one of the first choice SMOs due to its unique properties such as large band gap (3.37 eV), a high excitonic energy (60 meV) at room temperature, low resistivity, good thermal, mechanical and chemical stability.

➢ The Aims and Objectives:-

1) To study the growth of pure, Fe and Mg-doped zinc oxide nanostructured thin films prepared by using chemical spray pyrolysis technique.

2) To investigate the structural, morphological, optical, electrical, and gas sensing properties of Fe and Mg doped ZnO nanostructured thin films for improved applications in various field.

➢ Hypothesis of Research:-

The research work is directed to obtain Fe and Mg doped Zinc Oxide (ZnO) nanostructured thin films. In this study, the enhancement of structural, optical, morphological, and electrical properties of pure ZnO nanostructured thin films by doping of Fe and Mg will be expected. The gas sensing properties of the zinc oxide thin films will impact by the doping materials.

➢ Research Methodology:-

❖ Synthesis of good quality ZnO thin films:-

Spray pyrolysis is a process in which a thin film is deposited by spraying a solution on a heated surface, where the constituents react to form a chemical compound. It is proposed to grow pure, Fe and Mg doped zinc oxide nanostructured thin films by chemical spray pyrolysis technique and its different characterization can be studied. We use spray pyrolysis technique due to its adequate advantages like low cost, easy control of chemical uniformity, better stoichiometry control, easier fabrication of large area films and purity.

➢ Characterizations:-

1) Structural Characterization:-

X-Ray Diffraction:-

The powder X-Ray Diffraction (XRD) pattern will be recorded for pure, Fe and Mg-doped ZnO nanostructured Thin Films. The lattice constant, crystal structure, grain size and microstrain of the prepared samples will be studied.

2) **Morphological Characterization:-**

a) **Field Emission Scanning Electron Microscopy:-**

Field Emission Scanning Electron Microscopy (FE-SEM) is an advanced technology used to capture the microstructure image of the materials.

b) **Energy Dispersive X-Ray Analysis:-**

The compositional analysis of the prepared samples will be studied by Energy Dispersive X-Ray Analysis (EDAX).

3) **Optical Properties:-**

Synthesized samples of pure, Fe and Mg-doped ZnO nanostructured thin films will be characterized by UV-Visible Spectrophotometer. The obtained result will be used to calculate transparency and energy band gap of the prepared sample.

4) **Gas Sensing Properties** of Fe and Mg doped Zinc Oxide (ZnO) nanostructured thin films will be studied.

➢ Chapter Scheme:-

Chapter 1:- Introduction and Literature review

Chapter 2:- Experimental and Characterization techniques

Chapter 3:- Application based study of pure, Fe-doped ZnO nanostructured thin films

Chapter 4:- Application based study of pure, Mg-doped ZnO nanostructured thin films

Chapter 5:- Conclusions and scope for future.

➢ Year Wise Plan of Work and Targets to be achieved:-

First Year:-

- ❖ Course work
- ❖ Literature review
- ❖ Preparation of Fe-doped ZnO nanostructured thin films from chemical spray pyrolysis method.
- ❖ Structural, morphological, optical and gas sensing characterizations.

Second Year:-

- ❖ Preparation of Mg-doped ZnO nanostructured thin films from chemical spray pyrolysis method.
- ❖ Structural, morphological, optical and gas sensing characterizations.

Third Year:-

- ❖ Research paper publication on the work.
- ❖ Data analysis and the results obtained will be communicated to the respective journals for publication.
- ❖ Submission of the thesis for the Doctoral degree.

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